

# INFRARED SPECTROSCOPY

*By using IR Spectroscopy to identify functional group present in the compounds of 2-Mercaptodiphenylmethane and Sulphanilamide*

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**Abstract:** Absorption of radiation in the infrared region results in the excitation of bond deformations, either stretching or bending. Various stretching and bending vibrations occur at certain quantized frequencies. When infrared light of that frequency is incident on the molecule, energy is absorbed and the amplitude of that vibration is increased. By using various stretching and bending vibrations to identify C-S (str), C-H(str) and S-H(str) of 2-Mercaptodiphenylmethane, N-H (str), N-H (bend), SO<sub>2</sub> (str) and S-N Stretching of sulphanilamide.

**IndexTerm:** Stretching Vibrations, Bending Vibrations.

## I. INTRODUCTION

Infrared Spectroscopy is most useful technique detection of functional group present in the given compounds. Absorption of radiation in the infrared region results in the excitation of bond deformations, either stretching or bending. Various stretching and bending vibrations occur at certain quantized frequencies. When infrared light of that frequency is incident on the molecule, energy is absorbed and the amplitude of that vibration is increased.

An infrared spectrum is obtained when the frequency of molecular vibration corresponds to the frequency of the infrared radiation absorbed.

The material under study is usually in the form of a solid, a neat liquid or a solution. Sometimes, however, a compound in the gas or vapour phase is studied. Under these conditions, in addition to changes in vibrational energy, simultaneous changes in rotational energy can occur and consequently some fine structures may be observed on the vibrational band.

The normal range of an infrared spectrum, used by organic chemists for structural work, extends from 4000 cm<sup>-1</sup> to 667 cm<sup>-1</sup>. The shorter wavelength region (12500-4000 cm<sup>-1</sup>) is referred to as near infrared region and contains absorption bands due to harmonic overtones of fundamental bands and combination bands. The region extending from 667 cm<sup>-1</sup> to 50 cm<sup>-1</sup> is referred to as far infrared region. The normal and far infrared regions contain absorptions due to fundamental harmonic and combination bands.

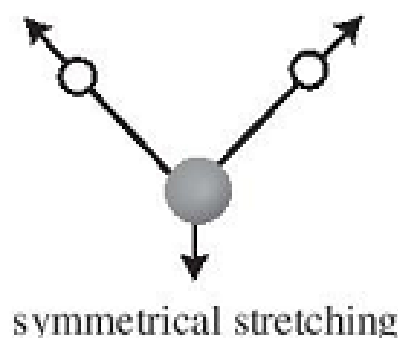
## II. STRETCHING AND BENDING VIBRATIONS

**Stretching Vibrations:** During Stretching vibrations, the distance between two atoms increases or decreases but the atoms remain in the same bond axis.

### TYPES OF STRETCHING VIBRATIONS

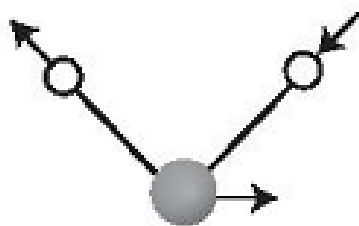
#### 1. Symmetrical stretching.

In this stretching mode, both the atoms move in and out simultaneously.



2. **Asymmetrical Stretching.**

In asymmetrical stretching, one atom moves in while the other moves out.

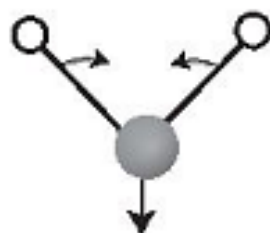


asymmetrical stretching

**BENDING VIBRATIONS (DEFORMATION)**

3. **In-plane scissoring deformation**

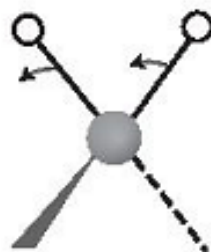
In the scissoring deformation mode, both the atoms swing in concert toward opposite directions.



scissoring (bending)

4. **In-plane rocking deformation.**

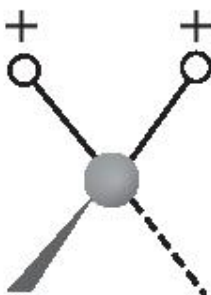
In this deformation mode, both the atoms swing to the same side and then both to the other side.



rocking, or bending in-plane

5. **Out-of-plane wagging deformation**

In this deformation mode, both the atoms swing up and down out of the plane of the paper.



wagging, or bending out-of-plane

## 6. Out-of-plane twisting deformation

In twisting deformation, one atom swings up and the other swings down.



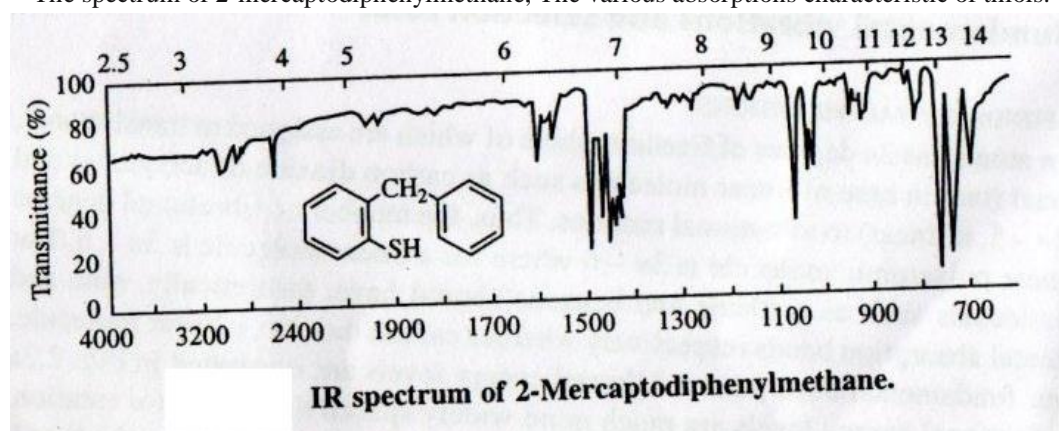
twisting, or bending out-of-plane

## SULPHIDES:

### C—S STRETCHING

The characteristic frequency for the C—S bond occurs between 700-600  $\text{cm}^{-1}$ . It is relatively weak and is not very satisfactory for analytical work because many compounds containing other functional groups or structures absorb more strongly in this region of the spectrum.

The spectrum of 2-mercaptodiphenylmethane, The various absorptions characteristic of thiols.



1. The weak absorption at 2930  $\text{cm}^{-1}$ , due to asymmetric  $\text{C}_{\text{sp}^3}$ -H stretching vibration, indicates the presence of methylene group. The absence of a methyl group is established by the absence of an absorption at 1380  $\text{cm}^{-1}$ .
2. The weak absorption at 3050  $\text{cm}^{-1}$  is due to aromatic C—H stretching vibration.
3. The sharp absorption at 2610  $\text{cm}^{-1}$  is due to an S—H stretching vibration.
4. The bands at 1603, 1585, 1570, 1451 and 1443  $\text{cm}^{-1}$  represent skeletal vibrations of an aromatic system. (The large number of absorptions between 1600 and 1400  $\text{cm}^{-1}$  suggests the presence of more than one benzene ring).
5. The absorption at 695 (aromatic C-C out of plane bending), 734 (aromatic C-H out-of-plane bending) and 760 (aromatic C-H out-of-plane bending, adjacent four H atoms) are characteristic substitution patterns for a monosubstituted and an ortho-disubstituted benzene ring systems.

## SULPHONAMIDES (-SO<sub>2</sub>-N<):

The various vibrations induced in sulphonamides along with their characteristic absorption frequencies are illustrated below:

### (a) N—H stretching vibrations

N—H asymmetric and symmetric stretching vibrations absorb near 3330 and 3260  $\text{cm}^{-1}$  respectively in primary sulphonamide, while a single band in the region 3300-3260  $\text{cm}^{-1}$  represents N—H stretching vibration in secondary sulphonamide.

### (b) N—H in-plane bending vibration

N—H in-plane bending vibration absorbs near 1570  $\text{cm}^{-1}$ .

### (c) SO<sub>2</sub> stretching vibrations

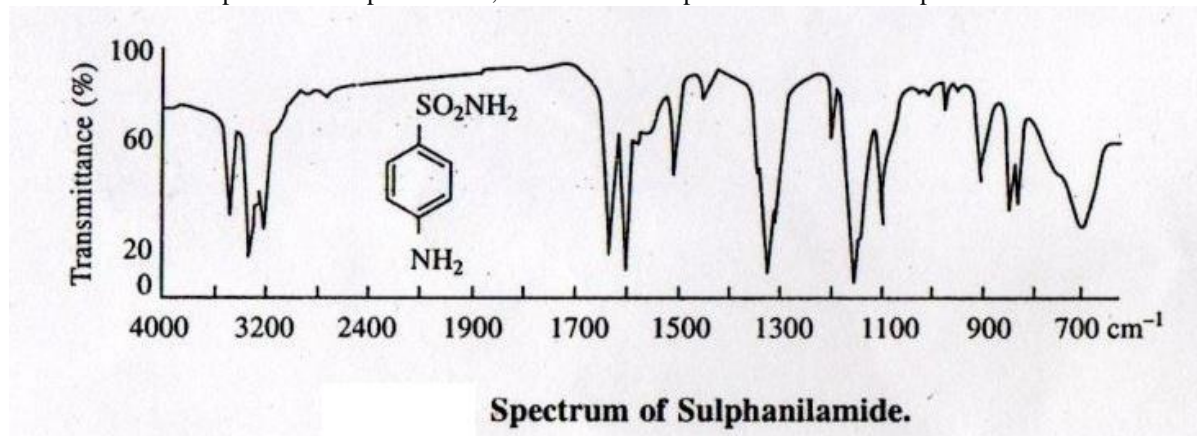
Asymmetric and symmetric SO<sub>2</sub> stretching vibrations appear as strong absorptions near 1370-1330 and 1180-1150  $\text{cm}^{-1}$  respectively. The fact that these S=O bands are observed at higher frequencies than in sulphones is contrary to the observed relation to C=O band in ketones and amides

### (d) S-N stretching vibrations

Sulphonamides exhibit S—N stretching vibrational frequency at 910-200  $\text{cm}^{-1}$

### Sulphanilamide

The spectrum of sulphanilamide, The various absorptions characteristic sulphonamides.



1. The absorptions at 3470 and 3320  $\text{cm}^{-1}$  are assigned respectively to asymmetric and symmetric N—H stretching vibrations of amino group. The corresponding N—H in-plane and out-of-plane bending vibrations occur at 1630 and 699  $\text{cm}^{-1}$  respectively.
2. The bands at 3260 and 3200  $\text{cm}^{-1}$  are due to asymmetric and symmetric N—H stretching vibrations of the sulphonamide group.
3. The absorptions at 1597 and 1504  $\text{cm}^{-1}$  represent the skeletal vibrations of the benzene ring.
4. The strong absorption at 1317  $\text{cm}^{-1}$  exhibits both asymmetric  $\text{SO}_2$  stretching and C—N stretching vibrations.
5. The strong absorption at 1149  $\text{cm}^{-1}$  suggests symmetric  $\text{SO}_2$  stretching vibration.
6. The medium intensity band at 902  $\text{cm}^{-1}$  is due to S—N stretching vibration.
7. The band at 839 or 829  $\text{cm}^{-1}$  is consistent with C—H out-of-plane bending vibration (two Adjacent hydrogen atoms) of p-disubstituted benzene ring.

### REFERENCES

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